

Energy spread and current-current correlation in quantum systems

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We consider energy (heat) transport in quantum systems, and establish a relationship between energy spread and energy current-current correlation function. The energy current-current correlation is related to thermal conductivity by the Green-Kubo formula, and thus this relationship allows us to study conductivity directly from the energy spread process. As an example, we investigate a spinless fermion model; the numerical results confirm the relationship.

I. INTRODUCTION

Heat transport has attracted increasing interest recently in both classical nonlinear lattices and quantum systems¹⁻⁵. In this field, a particularly interesting problem is related to the issue of Fourier's law. Considering for example the normal transport in one-dimensional systems, Fourier's law states that $j(x, t) = -\kappa \partial_x T(x, t)$, where $j(x, t)$ is the local heat current, $T(x, t)$ is the local equilibrium temperature, and κ is the heat conductivity. If we let $\varepsilon(x, t)$ denote the local energy density, then the continuity equation reads $\partial_t \varepsilon(x, t) + \partial_x j(x, t) = 0$. Combining these equations with $\frac{\partial \varepsilon}{\partial T} = c$, where c is the specific heat per unit volume, we arrive at the energy diffusion equation, $\partial_t \varepsilon(x, t) = \frac{\kappa}{c} \partial_x^2 \varepsilon(x, t)$.

In classical systems, it was shown that normal diffusion can be characterized by the mean squared displacement of the Helfand moment^{6,7}, which is related to the autocorrelation function of heat current and thus to the Green-Kubo formula. Beyond the normal diffusion, some recent works have investigated the relation between heat diffusion and conduction⁸⁻¹³. In particular, a rigorous relationship between energy (heat) spread and heat conduction has been established from statistical principles¹⁴. Therein, an excess energy distribution is introduced, and then the energy diffusion is characterized by the mean square deviation (MSD) of energy, which is connected to the autocorrelation function of heat current. Accordingly, how thermal conductivity depends on the system size may be extracted from energy diffusion in lattice systems^{10,15,16}.

Simultaneously, heat transport in low-dimensional quantum systems has also been investigated intensively¹⁷⁻²⁶. A commonly used method is the Green-Kubo formula within linear response theory, where nonzero Drude weights usually indicate ballistic transport. An interesting example is the ballistic energy transport in the spin- $\frac{1}{2}$ XXZ chain due to the conservation of the current operator²⁷⁻²⁹. Besides, quantum quench dynamics or spreading of different densities (e.g., energy densities) has also been studied³⁰⁻³². To determine whether the spread process is ballistical, diffusive, or of other type, one can observe the time evolution of the spatial variance σ^2 (or MSD) of certain nonequilibrium density. For ballistic transport, the variance behaviors as $\sigma^2 \sim t^2$ whereas for diffusive transport $\sigma^2 \sim t$. In Ref. 32, a connection between the variance and the current-autocorrelation function was proposed;

however, it is applicable at high temperatures. The general connection between the spreading processes and transport properties such as heat conductivity is not well understood yet.

In this paper, starting from an energy density distribution, we give a general connection between the MSD of energy diffusion and the autocorrelation function of energy current for quantum systems, within the linear response theory. This offers a different way to extract thermal conductivity from the energy spreading process. As an example, we apply it to a spinless fermion model, and the numerical results confirm this connection.

II. CONNECTION BETWEEN MSD AND CURRENT-AUTOCORRELATION FUNCTION

In the following, we restrict to the one-dimensional case. The generalization to higher-dimensional systems is straightforward. The system is typically described by a continuous Hamiltonian:

$$H_0 = \int h(x) dx. \quad (1)$$

At the infinite past an additional perturbation, $H' = -\int \eta(x) h(x) dx$, is also applied to the system. Here $\eta(x)$ is nonzero only in a local region. Thus the total Hamiltonian reads $H = H_0 + H'$. Before $t = 0$, we suppose the system is described by a canonical ensemble at temperature T . Then the partition function is $Z = \text{Tr}(e^{-\beta H})$, where $\beta = 1/k_B T$. At time $t = 0$, the perturbation is turned off suddenly. After that the quenched initial nonequilibrium state begins to relax towards the equilibrium state, and so does the local energy distribution. The local excess energy at $t > 0$ can be described by

$$\delta \langle h(x, t) \rangle_{neq} \equiv \langle h(x, t) \rangle_{neq} - \langle h(x) \rangle, \quad (2)$$

where $h(x, t) = e^{iH_0 t/\hbar} h(x) e^{-iH_0 t/\hbar}$. $\langle \cdot \rangle_{neq}$ denotes the expectation value in the nonequilibrium state, i.e., $\langle \cdot \rangle_{neq} = \text{Tr}(e^{-\beta H} \cdot) / Z$, and $\langle \cdot \rangle$ denotes the equilibrium average, $\langle \cdot \rangle = \text{Tr}(\rho_0 \cdot) / \text{Tr}(\rho_0)$ with $\rho_0 = e^{-\beta H_0} / \text{Tr}(e^{-\beta H_0})$.

To evaluate $\langle h(x, t) \rangle_{neq}$, we consider an operator $U(\tau) =$

$e^{H_0\tau/\hbar}e^{-H\tau/\hbar}$. The equation of motion of $U(\tau)$ is

$$-\hbar \frac{\partial U(\tau)}{\partial \tau} = H'(\tau)U(\tau), \quad (3)$$

where $H'(\tau) = e^{H_0\tau/\hbar}H'e^{-H_0\tau/\hbar}$. To the first order of H' , the solution can be written as $U(\tau) \approx 1 - \frac{1}{\hbar} \int_0^\tau d\tau' H'(\tau')$. Thus we may have

$$\begin{aligned} e^{-\beta H} &= e^{-\beta H_0} U(\hbar\beta) \\ &\approx e^{-\beta H_0} - \frac{1}{\hbar} e^{-\beta H_0} \int_0^{\hbar\beta} d\tau H'(\tau). \end{aligned} \quad (4)$$

Then we can obtain the partition function to the first order of H' ,

$$Z/Z_0 \approx 1 - \frac{1}{\hbar} \left\langle \int_0^{\hbar\beta} d\tau H'(\tau) \right\rangle. \quad (5)$$

Substituting Eqs. (4) and (5) into Eq. (2), we can obtain after some algebra,

$$\begin{aligned} \delta \langle h(x, t) \rangle_{neq} &= -\frac{1}{\hbar} \left\langle \int_0^{\hbar\beta} d\tau H'(\tau) h(x, t) \right\rangle \\ &+ \frac{1}{\hbar} \left\langle \int_0^{\hbar\beta} d\tau H'(\tau) \right\rangle \langle h(x, t) \rangle. \end{aligned} \quad (6)$$

The second term in Eq. (6) is time-independent actually. The probability distribution function is then defined as

$$\rho_E(x, t) = \delta \langle h(x, t) \rangle_{neq} / \mathcal{N}, \quad (7)$$

where $\mathcal{N} = \int dx \delta \langle h(x, t) \rangle_{neq} = Tc \int dx' \eta(x')$ is a normalization constant; see appendix A.

The mean square deviation for energy spread is then

$$\begin{aligned} \langle \Delta x^2(t) \rangle_E &\equiv \int (x - \langle x \rangle_E)^2 \rho_E(x, t) dx \\ &= \langle x^2(t) \rangle_E - \langle x \rangle_E^2. \end{aligned} \quad (8)$$

Using the reasoning similar to Ref. 14, it can be shown that $\langle x \rangle_E$ is a constant. For later convenience, we introduce two correlation functions:

$$C_{jj}(x't', xt) = \left\langle \int_0^{\hbar\beta} d\tau j(x', t' - i\tau) j(x, t) \right\rangle \quad (9)$$

and

$$C_{hh}(x't', xt) = \left\langle \int_0^{\hbar\beta} d\tau h(x', t' - i\tau) h(x, t) \right\rangle, \quad (10)$$

where the current operator $j(x, t)$ is defined via the continuity equation, $\partial_t h(x, t) + \partial_x j(x, t) = 0$. For homogeneous systems, these correlation functions are invariant under both temporal translation and spacial translation, i.e., $C_{jj}(x't', xt) = C_{jj}(x - x', t - t')$; a similar relation holds for C_{hh} . Further, we can have $\partial_t^2 C_{hh}(x't', xt) = \partial_x^2 C_{jj}(x't', xt)^{14}$.

Making use of the above equations, we can obtain

$$\begin{aligned} \mathcal{N} \frac{d^2 \langle x^2(t) \rangle_E}{dt^2} &= \frac{1}{\hbar} \int dx \int dx' x^2 \frac{d^2 C_{jj}(x'0, xt)}{dx^2} \eta(x') \\ &= \frac{1}{\hbar} \int dx x^2 \frac{d^2 C_{jj}(x, t)}{dx^2} \int dx' \eta(x'). \end{aligned} \quad (11)$$

That means

$$\frac{d^2 \langle x^2(t) \rangle_E}{dt^2} = \frac{1}{\hbar T c} \int dx x^2 \frac{d^2 C_{jj}(x, t)}{dx^2}. \quad (12)$$

Eq. (12) is a rigorous result. Integrating by parts twice and neglecting the boundary terms, we obtain the final result:

$$\frac{d^2 \langle x^2(t) \rangle_E}{dt^2} = \frac{2C_{JJ}(t)}{cT}, \quad (13)$$

where $C_{JJ}(t) = \lim_{L \rightarrow \infty} \frac{1}{L} \int_0^\beta d\lambda \langle J(-i\lambda\hbar) J(t) \rangle$ is the current-current correlation function that appears in the Green-Kubo formula for heat conductivity; see appendix B. Here $J = \int dx j(x)$ and L is the length of the system. It should be pointed out that taking the limit $L \rightarrow \infty$ is necessary, because in systems with a finite size the autocorrelation function $C_{jj}(x, t)$ at low temperatures may not decay to zero as x approaches to boundaries (see the example below). In that case, the boundary terms such as $C_{jj}(x, t)x|_{-L/2}^{L/2}$ need to be taken into account explicitly.

It is straightforward to extend Eq. (13) to other conserved quantities of the form $\hat{Q} = \int dx \hat{q}(x)$,

$$\frac{d^2 \langle x^2(t) \rangle_Q}{dt^2} = \frac{2C_{J_q J_q}(t)}{\beta \sigma_Q^2}, \quad (14)$$

where $\langle x^2(t) \rangle_Q$ is defined through the distribution $\delta \langle \hat{q}(x, t) \rangle_{neq}$, and $\sigma_Q^2 = (\langle \hat{Q}^2 \rangle - \langle \hat{Q} \rangle^2)/L$ is the fluctuation of quantity Q . The total current \hat{J}_q is given by $\hat{J}_q = \int dx \hat{j}_q(x)$, and $\hat{j}_q(x)$ is defined via the continuity equation $\partial_t \hat{q}(x, t) + \partial_x \hat{j}_q(x, t) = 0$. According to the time evolution of $\langle x^2(t) \rangle_Q$, transport processes may be classified as diffusive ($\langle x^2(t) \rangle_Q \sim t^\beta$, $\beta = 1$), super-diffusive ($1 < \beta \leq 2$), and sub-diffusive ($0 < \beta < 1$).

III. AN EXAMPLE: SPINLESS FERMION MODEL

As an application of Eq. (13), we consider a noninteracting fermion model, which may also be viewed as a spin- $\frac{1}{2}$ XY chain. For complicated systems, one may resort to methods such as finite-temperature, real-time density matrix renormalization group²². The Hamiltonian we consider reads

$$H_0 = -t_0 \sum_{i=-L/2+1}^{L/2} (c_i^\dagger c_{i+1} + \text{H.c.}) \equiv \sum_i h_i, \quad (15)$$

where h_i is the local energy operator. The total size of the system is L , and we adopt periodic boundary conditions. Via

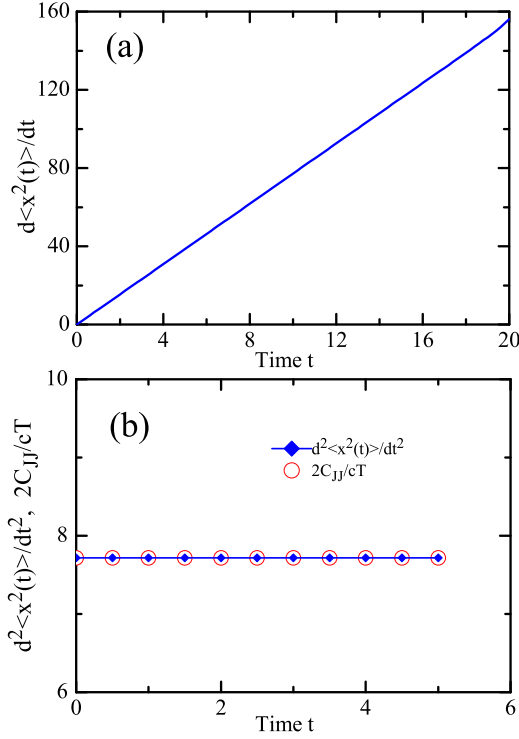


FIG. 1: (Color online) (a) The first derivative of the MSD with respect to time $d\langle x^2(t) \rangle_E / dt$ as a function of time. (b) Comparison of $\frac{d^2\langle x^2(t) \rangle_E}{dt^2}$ and $2C_{JJ}(t)/cT$. The parameters are $t_0 = 1$ and $T = 0.1$, and we choose $k_B = \hbar = 1$. The system size is $L = 100$.

the continuity equation, the current operator can be shown to be $j_i = \frac{it_0^2}{\hbar} (c_{i-1}^\dagger c_{i+1} - c_{i+1}^\dagger c_{i-1})$. The total energy current operator $J = \sum_i j_i$ commutes with H_0 , and thus is conserved. Note that usually energy current is different from heat current³³. However in the following we set the chemical potential to zero, so these two currents are the same in our case.

We assume a local perturbation, $H' = -\sum_i \eta_i h_i$, where $\eta_i = 0.2$ for $i = 0$ and $\eta_i = 0$ otherwise. To compute the MSD of energy diffusion, we first evaluate Eq. (6). In the basis of single-particle eigenstates of H_0 ($H_0|\alpha\rangle = \epsilon_\alpha|\alpha\rangle$), the operators can be expressed as

$$h_i(t) = \sum_{\alpha\beta} \langle \alpha | h_i | \beta \rangle c_\alpha^\dagger c_\beta e^{i(\epsilon_\alpha - \epsilon_\beta)t/\hbar} \quad (16)$$

and

$$H'(\tau) = \sum_{\alpha\beta} \langle \alpha | H' | \beta \rangle c_\alpha^\dagger c_\beta e^{i(\epsilon_\alpha - \epsilon_\beta)\tau/\hbar}, \quad (17)$$

where c_α^\dagger (c_α) creates (destroys) a particle occupying the state $|\alpha\rangle$. Substituting Eqs. (16) and (17) into Eq. (6), we can get after some algebra

$$\delta \langle h_i(t) \rangle_{neq} = \sum_{\alpha\beta} \langle \beta | H' | \alpha \rangle \langle \alpha | h_i | \beta \rangle e^{i(\epsilon_\alpha - \epsilon_\beta)t/\hbar} \frac{f_\alpha - f_\beta}{\epsilon_\alpha - \epsilon_\beta}, \quad (18)$$

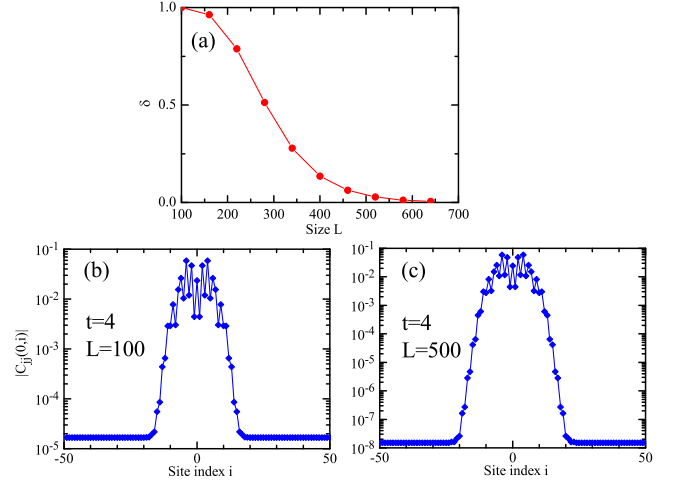


FIG. 2: (Color online) (a) Difference between the MSD of energy diffusion and $2C_{JJ}(t)/cT$ as a function of the system size. (b) and (c) $|C_{jj}(0, i)|$ in logarithm scale at time $t = 4$. In (b) the total size is $L = 100$ whereas in (c) $L = 500$. The temperature is $T = 0.01$. $k_B = \hbar = 1$.

where $f_\alpha = 1/(1 + e^{\epsilon_\alpha/k_B T})$ is the Fermi-Dirac distribution with the chemical potential being zero and we have used the identity $\text{Tr}[\rho_0 c_\beta^\dagger c_\alpha c_\gamma^\dagger c_\delta] = \delta_{\alpha\gamma} \delta_{\beta\delta} f_\beta (1 - f_\alpha) + \delta_{\alpha\beta} \delta_{\gamma\delta} f_\beta f_\gamma$. The specific heat can be easily evaluated from $C_V = \frac{\partial E}{\partial T}$, where $E = \sum_\alpha \epsilon_\alpha f_\alpha$. In a similar way we can evaluate $C_{JJ}(t)$, and the final result is

$$C_{JJ}(t) = -\frac{1}{L} \sum_{\alpha\beta} \langle \beta | \hat{J} | \alpha \rangle \langle \alpha | \hat{J} | \beta \rangle \times \frac{f_\alpha - f_\beta}{\epsilon_\alpha - \epsilon_\beta} e^{i(\epsilon_\alpha - \epsilon_\beta)t/\hbar}. \quad (19)$$

In numerical simulations, we take $t_0 = 1$ as units of energy, and we set $k_B = \hbar = 1$. In Fig. 1(a), we plot the first derivative of $\langle x^2(t) \rangle_E$ with respect to time at a high temperature $T = 0.1$. The corresponding real temperature is of order 10^3 K, and a finite size $L = 100$ is used here. We see that $d\langle x^2(t) \rangle_E / dt$ linearly increases with time. This is also reflected in Fig. 1(b), where $\frac{d^2\langle x^2(t) \rangle_E}{dt^2}$ is clearly a constant. Thus the transport process is ballistic. To check the validity of Eq. (13), we plot $\frac{d^2\langle x^2(t) \rangle_E}{dt^2}$ and $2C_{JJ}(t)/cT$ as functions of time in Fig. 1(b), and a good agreement can be observed.

At low temperatures, the finite size effect becomes prominent; i.e., there could be a big difference between $\frac{d^2\langle x^2(t) \rangle_E}{dt^2}$ and $2C_{JJ}(t)/cT$ when the system size is not large enough. To characterize this difference, we plot the relative error

$$\delta = \left| \frac{d^2\langle x^2(t) \rangle_E}{dt^2} - \frac{2C_{JJ}(t)}{cT} \right| / \left| \frac{d^2\langle x^2(t) \rangle_E}{dt^2} \right| \quad (20)$$

in Fig. 2(a). As the size increases, the error δ decays to zero rapidly. The reason for the big difference at a small size is that the current autocorrelation function $C_{jj}(x' = 0, x = i)$ does not decay to zero at the boundaries. For $L = 100$, $C_{jj}(0, i)$

takes an appreciably small value at the boundaries, while $C_{jj}(0, i)$ becomes very small at the boundaries for $L = 500$; see Figs. 2(b) and (c). Thus when integrating Eq. (12) to get Eq. (13), we can not neglect the boundary terms for small systems. When the boundary terms are taken into account, we have found excellent agreement between $\frac{d^2\langle x^2(t) \rangle_E}{dt^2}$ and $2C_{JJ}(t)/cT$ plus boundary terms regardless of the system size.

IV. CONCLUSIONS

In summary, within the linear response theory we have established a connection between the MSD of energy diffusion and the autocorrelation function of energy current for quantum systems, i.e., $\frac{d^2\langle x^2(t) \rangle_E}{dt^2} = \frac{2C_{JJ}(t)}{cT}$. It is straightforward to extend it to other conserved quantities. As an example, we have applied it to a spinless fermion model (or the spin-1/2 XY model). We found that at high temperatures $\frac{d^2\langle x^2(t) \rangle_E}{dt^2}$ is consistent with $2C_{JJ}(t)/cT$ even for a comparatively small size $L = 100$. However, at low temperatures, there may be large difference between $\frac{d^2\langle x^2(t) \rangle_E}{dt^2}$ and $2C_{JJ}(t)/cT$ when the system size is small due to the ignorance of boundary terms. Indeed when the boundary terms are included, we could still find excellent agreement between $\frac{d^2\langle x^2(t) \rangle_E}{dt^2}$ and $2C_{JJ}(t)/cT$ plus boundary terms regardless of the system size. This connection thus offers an alternative way to extract conductivity from the energy spreading process in quantum systems.

Acknowledgments

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Appendix A: Normalization constant

Here we will show $\mathcal{N} = \int dx \delta\langle h(x, t) \rangle_{neq} = Tc \int dx' \eta(x')$. From Eq. (6), we see that \mathcal{N} consists of two terms. The first term is

$$\begin{aligned} & -\frac{1}{\hbar} \int dx \langle \int_0^{\hbar\beta} d\tau H'(\tau) h(x, t) \rangle \\ &= \frac{1}{\hbar} \int dx \int dx' \langle \int_0^{\hbar\beta} d\tau h(x', \tau) h(x, t) \rangle \eta(x') \\ &= \frac{1}{\hbar} \langle \int_0^{\hbar\beta} d\tau h(0, \tau) H_0 \rangle \int dx' \eta(x') \\ &= \frac{1}{\hbar L} \int dy \langle \int_0^{\hbar\beta} d\tau h(y, \tau) H_0 \rangle \int dx' \eta(x') \\ &= \frac{\beta}{L} \langle H_0^2 \rangle \int dx' \eta(x'), \end{aligned} \quad (A1)$$

where we have used the spacial-translation invariance of $C_{hh}(x'0, xt)$. The second term is

$$\begin{aligned} & \frac{1}{\hbar} \langle \int_0^{\hbar\beta} d\tau H'(\tau) \rangle \langle h(x, t) \rangle \\ &= -\frac{1}{\hbar} \int dx' \langle \int_0^{\hbar\beta} d\tau h(x', \tau) \rangle \eta(x') \langle H_0 \rangle \\ &= -\frac{1}{\hbar} \langle \int_0^{\hbar\beta} d\tau h(0, \tau) \rangle \langle H_0 \rangle \int dx' \eta(x') \\ &= -\frac{1}{\hbar L} \int dy \langle \int_0^{\hbar\beta} d\tau h(y, \tau) \rangle \langle H_0 \rangle \int dx' \eta(x') \\ &= -\frac{\beta}{L} \langle H_0 \rangle^2 \int dx' \eta(x'). \end{aligned} \quad (A2)$$

Upon combining these two terms, we have $\mathcal{N} = \frac{\beta}{L} [\langle H_0^2 \rangle - \langle H_0 \rangle^2] \int dx' \eta(x')$. From $C_V = \frac{\partial E}{\partial T}$, where $E = \text{Tr}(e^{-\beta H_0} H_0) / \text{Tr}(e^{-\beta H_0})$, we can obtain $\langle H_0^2 \rangle - \langle H_0 \rangle^2 = TC_V / \beta$. So we have

$$\mathcal{N} = Tc \int dx' \eta(x'). \quad (A3)$$

Appendix B: Green-Kubo formula for heat conductivity

Here we give a very brief introduction to the Green-Kubo formula. We begin with the following partition function,

$$Z_0 = \text{Tr}[e^{-\beta H_0}]. \quad (B1)$$

Applying a temperature gradient across the system [$T(x) = T + \delta T(x)$] and assuming local equilibrium, then we may expect

$$\begin{aligned} \beta H_0 &\rightarrow \beta \int dx h(x) [1 - \frac{\delta T(x)}{T}] \\ &= \beta [\int dx h(x) - \int dx h(x) \frac{\delta T(x)}{T}]. \end{aligned} \quad (B2)$$

We can treat the second term as a perturbation

$$H' = - \int dx h(x) \frac{\delta T(x)}{T} \equiv \hat{F}. \quad (B3)$$

Then within the linear response theory the heat current can be written as³³

$$\begin{aligned} j(x) &= \int_{-\infty}^0 dt e^{\eta t} \int_0^{\beta} d\lambda \\ &\quad \times \text{Tr}[\rho_0 \int dx' j(x', t - i\lambda\hbar) j(x) \frac{1}{T} \frac{\partial \delta T}{\partial x'}], \end{aligned} \quad (B4)$$

where $\eta = 0^+$ and $\rho_0 = e^{-\beta H_0} / Z_0$. Assuming a uniform temperature gradient [$\frac{\partial \delta T}{\partial x'} = \text{const.}$], we thus obtain heat conductivity:

$$\begin{aligned} \kappa &= \text{Re} \left\{ \frac{1}{LT} \int_0^{\infty} dt e^{-\eta t} \int_0^{\beta} d\lambda \text{Tr}[\rho_0 J(-t - i\lambda\hbar) J] \right\} \\ &= \text{Re} \left\{ \frac{1}{T} \int_0^{\infty} dt e^{-\eta t} C_{JJ}(t) \right\}, \end{aligned} \quad (B5)$$

where $J = \int dx j(x)$ and

$$C_{JJ}(t) = \lim_{L \rightarrow \infty} \frac{1}{L} \langle \int_0^\beta d\lambda J(-i\lambda\hbar) J(t) \rangle. \quad (\text{B6})$$

The above equation may also be cast in the following form

$$\kappa = \frac{1}{Lk_B T^2} \frac{1}{2} \int_0^\infty dt \langle \{J, J(t)\} \rangle, \quad (\text{B7})$$

which can be shown in the basis of eigenstates of H_0 . Although the Green-Kubo formula for heat conductivity is questionable, we will not go into the details here^{3,34}.

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